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On Solving Large-Scale Free Material Optimization Problems

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On Solving Large-Scale Free Material Optimization Problems

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Free Material Optimization (FMO)

- The design variable is the entire material tensor $\boldsymbol{E}$

$$\boxed{\boldsymbol{\sigma}_{ij}(x) = \boldsymbol{E}_{ijkl}(x)\boldsymbol{e}_{kl}(x)}$$

  - allowed to vary freely at each point of the design domain
  - the only requirement is that the material tensors should be symmetric and positive semidefinite

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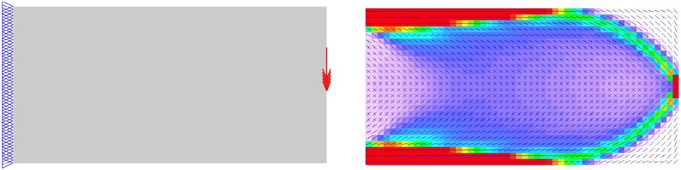

  - obtains conceptual optimal structures regarded as ultimately best designs.
  - can be used to generate benchmark solutions for other models and besides to propose novel ideas for new design situations.

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Motivation

FMO problems

- demand fine finite element discretization, hence large problems
- involve matrix inequities/variables
- are modeled as nonlinear (mostly non convex) semidefinite programming
- are computationally expensive and more difficult than standard optimization problems.

Most today's methods are based on first-order method leading to many iterations.

Objective

- To develop special purpose second order interior point method that can robustly and efficiently solve large-scale FMO problems.

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- To develop special purpose second order interior point method that can robustly and efficiently solve large-scale FMO problems.
- To investigate numerically the performance of
    - some equivalent FMO problem formulations
    - the most common directions (AHO, HRVW/KSH/M, and NT directions) for solving FMO problems.

Primal problems (SAND)

Minimum compliance

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, \boldsymbol{E} \in \mathbb{E}}{\text{minimize}} \quad & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E}) \boldsymbol{u}_\ell = \boldsymbol{f}_\ell, \ \ell \in L, \\ & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \leq V. \end{aligned}$$

where the discrete set of admissible materials

$$\boxed{\mathbb{E} := \left\{ \boldsymbol{E} \in (\mathbb{R}^{dm \times d}) | \boldsymbol{E}_i = \boldsymbol{E}_i^T \succeq 0, \underline{\rho} \leq Tr(\boldsymbol{E}_i) \leq \bar{\rho}, i = 1, \ldots, m \right\}}$$

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Minimum weight

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, E \in \boldsymbol{E}}{\text{minimize}} \quad & \sum_{i=1}^m Tr(\boldsymbol{E}_i) \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E})\boldsymbol{u}_\ell = \boldsymbol{f}_\ell, \ \ell \in \mathcal{L}, \\ & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \leq \gamma, \end{aligned}$$

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Primal problems (Nested)

Minimum compliance

$$\begin{aligned} \underset{\boldsymbol{E}\in\mathbb{E}}{\text{minimize}} \quad & \sum_{\ell\in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{A}^{-1}(\boldsymbol{E})\boldsymbol{f}_\ell \\ \text{subject to} \quad & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \leq V. \end{aligned}$$

Minimum weight

$$\begin{aligned} \underset{\boldsymbol{E}\in\mathbb{E}}{\text{minimize}} \quad & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \\ \text{subject to} \quad & \sum_{\ell\in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{A}^{-1}(\boldsymbol{E})\boldsymbol{f}_\ell \leq \gamma \end{aligned}$$

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Primal problems (Linear)

Primal problems (Linear)

Minimum compliance

$$\begin{aligned} \underset{\boldsymbol{E}\in\mathbb{E},\varrho_\ell\geq 0}{\text{minimize}} \quad & \sum_{\ell\in L} w_\ell \varrho_\ell \\ \text{subject to} \quad & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \leq V, \\ & \begin{pmatrix} \varrho_\ell & \boldsymbol{f}_\ell^T \\ \boldsymbol{f}_\ell & \boldsymbol{A}(\boldsymbol{E}) \end{pmatrix} \succeq 0, \ \forall \ell \in L. \end{aligned}$$

Minimum weight

$$\begin{aligned} \underset{\boldsymbol{E}\in\mathbb{E},\tau_\ell\geq 0}{\text{minimize}} \quad & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \\ \text{subject to} \quad & \sum_{\ell\in\mathcal{L}} w_\ell \tau_\ell \leq \bar{\gamma}, \\ & \begin{pmatrix} \tau_\ell & \boldsymbol{f}_\ell^T \\ \boldsymbol{f}_\ell & \boldsymbol{A}(\boldsymbol{E}) \end{pmatrix} \succeq 0, \ \forall \ell \in \mathcal{L}. \end{aligned}$$

$$\boxed{\mathbb{E} := \left\{ \boldsymbol{E} \in (\mathbb{R}^{dm\times d}) | \boldsymbol{E}_i = \boldsymbol{E}_i^T \succeq 0, \underline{\rho} \leq Tr(\boldsymbol{E}_i) \leq \bar{\rho}, i = 1, \ldots, m \right\}}$$

Very large-scale matrix inequalities which are difficult to deal within computations.

Dual problems

The minimum compliance primal problem

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, \boldsymbol{E}}{\text{minimize}} \quad & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E})\boldsymbol{u}_\ell = \boldsymbol{f}_\ell, \ \ell \in L, \\ & \boldsymbol{E}_i = \boldsymbol{E}_i^T \succeq 0, \ i = 1, \dots, m, \\ & \underline{\rho} \leq Tr(\boldsymbol{E}_i) \leq \bar{\rho}, \ i = 1, \dots, m, \\ & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \leq V. \end{aligned}$$

has the dual problem given by

$$\begin{aligned} \underset{\substack{\boldsymbol{u}_1, \dots, \boldsymbol{u}_{n_L} \in \mathbb{R}^n \\ \alpha \in \mathbb{R}, \bar{\beta} \in \mathbb{R}^m, \underline{\beta} \in \mathbb{R}^m}}{\text{maximize}} \quad & -\alpha \bar{V} + 2 \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell + \underline{\rho} \sum_{i=1}^{m} \underline{\beta}_i - \bar{\rho} \sum_{i=1}^{m} \bar{\beta}_i \\ \text{subject to} \quad & \sum_{\ell \in L} \sum_{k=1}^{n_G} w_\ell \boldsymbol{B}_{i,k}^T \boldsymbol{u}_\ell \boldsymbol{u}_\ell^T \boldsymbol{B}_{i,k} - (\alpha - \underline{\beta}_i + \bar{\beta}_i)\boldsymbol{I} \preceq 0 \, , i = 1, \dots, m \\ & \alpha \geq 0, \bar{\beta} \geq 0, \underline{\beta} \geq 0. \end{aligned}$$

Primal and dual problems

Minimum complinace problems (SAND, Nested, and Dual)

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, \boldsymbol{E} \in \mathbb{E}}{\text{minimize}} \quad & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E}) \boldsymbol{u}_\ell = \boldsymbol{f}_\ell, \ \ell \in L, \\ & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \leq V. \end{aligned}$$

$$\begin{aligned} \underset{\boldsymbol{E} \in \mathbb{E}}{\text{minimize}} \quad & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{A}^{-1}(\boldsymbol{E}) \boldsymbol{f}_\ell \\ \text{subject to} \quad & \sum_{i=1}^{m} Tr(\boldsymbol{E}_i) \leq V. \end{aligned}$$

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Minimum weight problems (SAND and Nested)

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, \boldsymbol{E} \in \mathbb{E}}{\text{minimize}} \quad & \sum_{i=1}^m Tr(\boldsymbol{E}_i) \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E})\boldsymbol{u}_\ell = \boldsymbol{f}_\ell,\ \ell \in \mathcal{L}, \\ & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \le \gamma, \end{aligned}$$

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Primal-dual interior point method

Consider the nonlinear semidefinite problem

$$\boxed{\begin{array}{lll} \underset{\boldsymbol{X}\in\mathbb{S},\boldsymbol{u}\in\mathbb{R}^n}{\text{minimize}} & f(\boldsymbol{X},\boldsymbol{u}) & \\ \text{subject to} & g_j(\boldsymbol{X},\boldsymbol{u}) \leq 0, & j=1,\ldots,k, \\ & \boldsymbol{X}_i \succeq 0, & i=1,\ldots m, \end{array}} \qquad \text{(P)}$$

where, $\mathbb{S} = \mathbb{S}^{d_1} \times \mathbb{S}^{d_2} \times \cdots \times \mathbb{S}^{d_m}$ and $(d_1, d_2, \ldots, d_m) \in \mathbb{N}^m$,.

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where, $\mathbb{S} = \mathbb{S}^{d_1} \times \mathbb{S}^{d_2} \times \cdots \times \mathbb{S}^{d_m}$ and $(d_1, d_2, \dots, d_m) \in \mathbb{N}^m$,.

We introduce the slack variables $\boldsymbol{s} \in \mathbb{R}^k$ and barrier parameter $\mu > 0$ and formulate the associated barrier problem as

$$\begin{array}{ll} \underset{\boldsymbol{X}\in\mathbb{S}_+,\boldsymbol{u}\in\mathbb{R}^n,\boldsymbol{s}\in\mathbb{R}^k_+}{\text{minimize}} & f(\boldsymbol{X},\boldsymbol{u}) - \mu\sum_{i=1}^{m}\ln(\det(\boldsymbol{X}_i)) - \mu\sum_{j=1}^{k}\ln(s_j) \\ \text{subject to} & g_j(\boldsymbol{X},\boldsymbol{u}) + s_j = 0, \quad j=1,\dots,k. \end{array} \tag{BP}$$

The central idea in interior point methods is that to solve the barrier problem (BP) for a sequence of barrier parameter $\mu_k \to 0$

Optimality conditions

The first-order optimality conditions of the barrier problem (BP) are

$$\begin{pmatrix} \nabla_{\boldsymbol{X}} f(\boldsymbol{X}, \boldsymbol{u}) - \boldsymbol{Z} + \nabla_{\boldsymbol{X}}(g(\boldsymbol{X}, \boldsymbol{u})^T \boldsymbol{\lambda}) \\ \nabla_{\boldsymbol{u}} f(\boldsymbol{X}, \boldsymbol{u}) + \nabla_{\boldsymbol{u}} g(\boldsymbol{X}, \boldsymbol{u})^T \boldsymbol{\lambda} \\ \boldsymbol{S}\boldsymbol{\Lambda}\boldsymbol{e} - \mu\boldsymbol{e} \\ g(\boldsymbol{X}, \boldsymbol{u}) + \boldsymbol{s} \\ \color{red}{\boldsymbol{X}\boldsymbol{Z} - \mu\boldsymbol{I}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

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$$\begin{pmatrix} \nabla_{\boldsymbol{X}} f(\boldsymbol{X},\boldsymbol{u}) - \boldsymbol{Z} + \nabla_{\boldsymbol{X}} (g(\boldsymbol{X},\boldsymbol{u})^T \boldsymbol{\lambda}) \\ \nabla_{\boldsymbol{u}} f(\boldsymbol{X},\boldsymbol{u}) + \nabla_{\boldsymbol{u}} g(\boldsymbol{X},\boldsymbol{u})^T \boldsymbol{\lambda} \\ \boldsymbol{S}\boldsymbol{\Lambda}\boldsymbol{e} - \mu \boldsymbol{e} \\ g(\boldsymbol{X},\boldsymbol{u}) + \boldsymbol{s} \\ H_P(\boldsymbol{X}\boldsymbol{Z}) - \mu \boldsymbol{I} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

where
$H_{\boldsymbol{P}} : \mathbb{R}^{n\times n} \to \mathbb{S}^n$, defined by $H_{\boldsymbol{P}}(\boldsymbol{Q}) := \frac{1}{2}\left(\boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^{-1} + (\boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^{-1})^T\right)$.

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- $\boldsymbol{P} = \boldsymbol{I}$, AHO direction
- $\boldsymbol{P} = \boldsymbol{Z}^{1/2}$, HRVW/KSH/M direction **(H.K.M.)**
- $\boldsymbol{P} = \boldsymbol{X}^{-1/2}$, dual HRVW/KSH/M direction
- $\boldsymbol{P} = \boldsymbol{W}^{-1/2}$, NT direction
  $\boldsymbol{W} = \boldsymbol{X}^{1/2}(\boldsymbol{X}^{1/2}\boldsymbol{Z}\boldsymbol{X}^{1/2})^{-1/2}\boldsymbol{X}^{1/2}$

Applying Newton's method we solve the reduced system

$$\boxed{\begin{pmatrix} \boldsymbol{G} & \boldsymbol{A} \\ \boldsymbol{A}^T & \boldsymbol{B} \end{pmatrix} \begin{pmatrix} \Delta \boldsymbol{u} \\ \Delta \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \tilde{\boldsymbol{r}}_d \\ \tilde{\boldsymbol{r}}_p \end{pmatrix}}$$

$$\boldsymbol{G} = \boldsymbol{G}(\tilde{\boldsymbol{H}}^{-1}), \boldsymbol{A} = \boldsymbol{A}(\tilde{\boldsymbol{H}}^{-1}), \boldsymbol{B} = \boldsymbol{B}(\tilde{\boldsymbol{H}}^{-1})$$

$$\tilde{\boldsymbol{r}}_d = \tilde{\boldsymbol{r}}_d(\tilde{\boldsymbol{H}}^{-1}), \tilde{\boldsymbol{r}}_p = \tilde{\boldsymbol{r}}_p(\tilde{\boldsymbol{H}}^{-1})$$

$$\boxed{\tilde{\boldsymbol{H}} = \nabla^2_{\boldsymbol{X}\boldsymbol{X}} \mathcal{L}_\mu(\boldsymbol{X}, \boldsymbol{u}, \boldsymbol{s}, \boldsymbol{\lambda}) + \mathcal{F}^{-1}\mathcal{E}}$$

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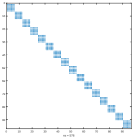

The other search directions $(\boldsymbol{\Delta} X, \Delta \boldsymbol{s}, \Delta \boldsymbol{Z})$ are then determined

Problem formulations

Minimum complinace problems (SAND, Nested, and Dual)

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, \boldsymbol{E} \in \mathbb{E}}{\text{minimize}} \quad & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E}) \boldsymbol{u}_\ell = \boldsymbol{f}_\ell, \ \ell \in L, \\ & \sum_{i=1}^m Tr(\boldsymbol{E}_i) \le V. \end{aligned}$$

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Minimum weight problems (SAND and Nested)

$$\begin{aligned} \underset{\boldsymbol{u}_\ell \in \mathbb{R}^n, \boldsymbol{E} \in \mathbb{E}}{\text{minimize}} \quad & \sum_{i=1}^m Tr(\boldsymbol{E}_i) \\ \text{subject to} \quad & \boldsymbol{A}(\boldsymbol{E}) \boldsymbol{u}_\ell = \boldsymbol{f}_\ell, \ \ell \in \mathcal{L}, \\ & \sum_{\ell \in L} w_\ell \boldsymbol{f}_\ell^T \boldsymbol{u}_\ell \le \gamma, \end{aligned}$$

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2D problems

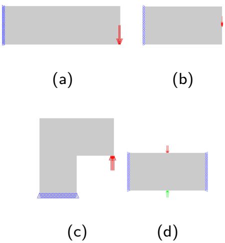
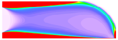


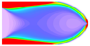
Figure: Design domains, boundary conditions, and external loads for the Cantilever benchmark problem (a), the Michell beam problem (b), the L-shape problem (c), and the two load case problem (d).

Problem instances		
Problems	No. of finite elements	No. of design variables
Cantilever I	7500	45000
Cantilever II	30000	180000
Cantilever III	120000	720000
Cantilever IV	480000	2880000
Michell I	5000	30000
Michell II	20000	120000
Michell III	80000	480000
Michell IV	320000	1920000
L-shape I	1875	11250
L-shape II	7500	45000
L-shape III	30000	180000
L-shape IV	120000	720000
Two Loads case I	5000	30000
Two Loads case II	20000	120000
Two Loads case III	80000	480000
Two Loads case IV	320000	1920000

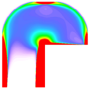
Optimal designs and numerical results



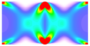
(a)



(b)



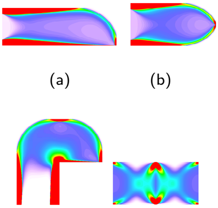
(c)



(d)

Figure: Optimal density distributions obtained by solving the minimum compliance problem for the Cantilever IV benchmark problem (a), the Michell IV beam problem (b), the L-shape IV problem (c), and the two load case IV problem (d).

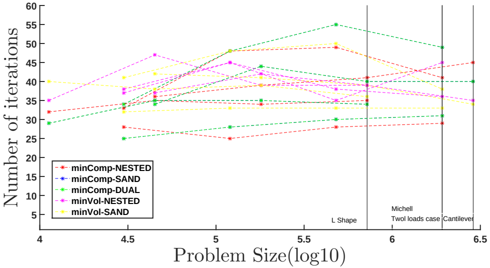
Optimal designs and numerical results



(a) (b)

(c) (d)

Figure: Optimal density distributions obtained by solving the minimum compliance problem for the Cantilever IV benchmark problem (a), the Michell IV beam problem (b), the L-shape IV problem (c), and the two load case IV problem (d).



Optimal designs and numerical results

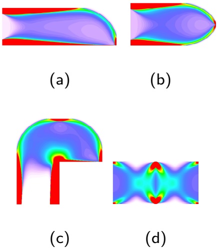
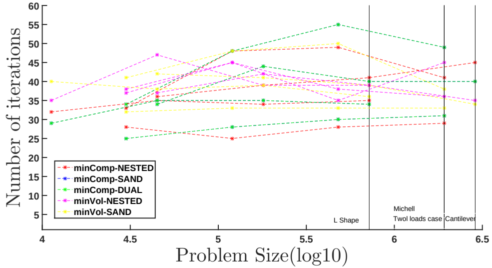
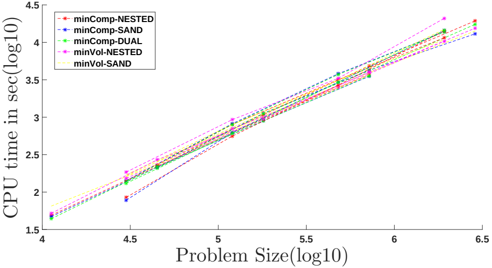
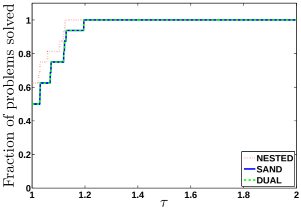


Figure: Optimal density distributions obtained by solving the minimum compliance problem for the Cantilever IV benchmark problem (a), the Michell IV beam problem (b), the L-shape IV problem (c), and the two load case IV problem (d).

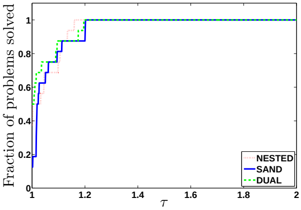




Numerical results/problem formulations



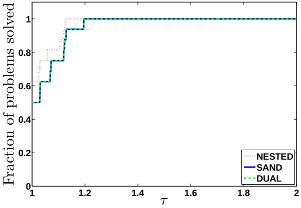
(a) Number of iterations as performance measure



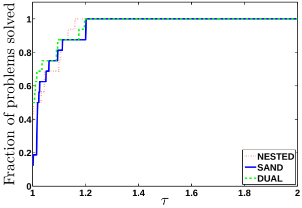
(b) CPU time as performance measure

Figure: Performance profiles for the minimum compliance problem.

Numerical results/problem formulations

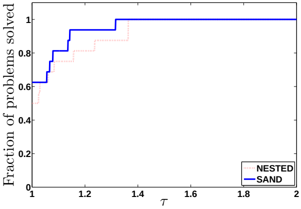


(a) Number of iterations as performance measure

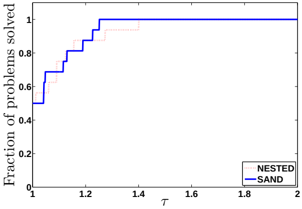


(b) CPU time as performance measure

Figure: Performance profiles for the minimum compliance problem.



(a) Number of iterations as performance measure



(b) CPU time as performance measure

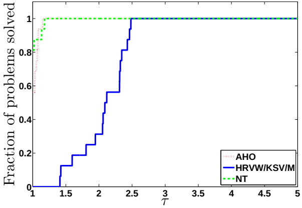
Figure: Performance profiles for the minimum weight problem.

Numerical results/search directions

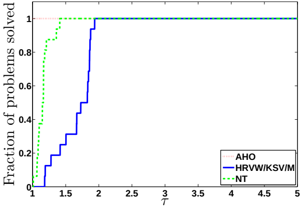
Moreover, we compare the numerical performance of the

- AHO direction
- HRVW/KSH/M direction
- NT direction

for solving the minimum compliance problem of the SAND formulation.



(a) Number of iterations as performance measure



(b) CPU time as performance measure

Figure: Performance profiles for the search directions.

Conclusions

- Efficient second order primal-dual interior point for FMO is developed.
- The method requires modest number of iterations and almost independent of problem size.
- The method has obtained solutions of good quality to the largest FMO problems to date.
- There is no clear distinction in the performance of the standard FMO problem formulations.
- We recommend the NT direction for solving FMO problems for its efficiency and robustness .

A. G. Weldeyesus and M. Stolpe. A primal-dual interior point method for large-scale free material optimization. *Computational Optimization and Applications*, 61(2):409–435, 2015.

Thank you for your attention!